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A scale-adaptive framework to predict water and nutrient fluxes across land-water interfaces

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Watershed hydrobiogeochemical models informed by multiple data layers are essential to quantifying water and nutrient fluxes across land-water interfaces and predicting downstream river water quality. However, scale-adaptive numerical methods are needed to enable the appropriate representation of multi-scale, multi-physics watershed processes. Here, we present a scale-adaptive reactive transport simulation framework that melds process fidelity with computational tractability. We conducted this work in the East River Mountainous Watershed in Colorado, a study site of Berkeley Lab's Watershed Function Scientific Focus Area. To compute water and nutrient fluxes across land-water interfaces, we modeled a 10-meander region of the East River Floodplain using PFLOTRAN, a process-rich, open-source, high-performance simulator. We developed the RiverFlotran Module and integrated that with PFLOTRAN. The RiverFlotran module uses the fully dynamic 1D shallow-water equations. For the hydrodynamics in the river, we solve the fully dynamic shallow water equations in one dimension. Using the 10-meander model, we developed relationships between hydrobiogeochemical exchanges and the characteristic watershed features such as topography, wetness index, meanders, sinuosity, and amplitudes to quantify subsurface geochemical exports. The results show that because of prevailing anoxic conditions in the alluvial aquifer of the East River Floodplain, dissolved iron and nitrogen profiles exhibit strong redox gradients in the subsurface and are exported back to the stream on the downstream side of meanders. We further noted that meander bends are hot spots of nitrogen species, irrespective of high and low water-level conditions. We found that these nitrogen hot spots are produced due to spatial and temporal variations in the river stage, bathymetry, and meander geometry (e.g., sinuosity). Our modeling framework sets the stage to quantify river water quality at the watershed scale. Efforts are underway to integrate hydrobiogeochemical exchanges using advanced machine learning techniques with the East River Watershed's large drainage network.